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*Department of Physics, Erevan State University*[1]) *(a)*
*and I. V. Kurchatov Institute of Atomic Energy, Moscow (b)*

# A New Type of Monochromator for Synchrotron Radiation with Three-Wave Bragg Diffraction

By

R. Z. GABRIELYAN (a) and V. G. KOHN (b)

A new set-up of a crystal monochromator with three-wave Bragg diffraction, which permits to realize a four-crystal spectrometer in a relatively simple way is offered. Instead of three initial crystals, three sets of reflecting planes from the same crystal are used. The crystal monochromator, consisting of three blocks on a common basis and using the symmetric Bragg three-wave coplanar scattering is described in detail. A calculation of the angular and spectral characteristics of the crystal monochromator in the case (044/440) of three-wave diffraction in silicon is carried out. The calculation shows that the considered set-up of reflecting surface blocks is highly effective.

Ein neuer Aufbau eines Kristallmonochromators mit Dreiwellen-Braggbeugung wird mitgeteilt, der es erlaubt, in relativ einfacher Weise ein Vierkristallspektrometer zu realisieren. Statt dreier Kristalle werden drei Sätze reflektierender Ebenen von demselben Kristall benutzt. Der Kristallmonochromator, bestehend aus drei Blöcken auf einer gemeinsamen Basis und unter Benutzung der symmetrischen, koplanaren Braggschen Dreiwellen-Streuung, wird ausführlich beschrieben. Eine Berechnung der Winkel- und Spektralcharakteristiken des Kristallmonochromators wird für den Fall (044/440) der Dreiwellen-Beugung in Silizium durchgeführt. Die Rechnung zeigt, daß der betrachtete Aufbau von reflektierenden Oberflächenblöcken sehr wirkungsvoll ist.

Synchrotron radiation is known to have a continuous spectrum and for its effective use in studies of perfect crystals it is necessary to carry out preliminary accurate monochromatization and collimation. Due to the weak interaction between the electromagnetic X-radiation and the crystal, the diffracted wave intensity has an appreciable magnitude only at angles of incidence differing from the Bragg angle by no more than some 10″ and at fixed angle of incidence for which the ratio $\Delta\omega/\omega \leqq \leqq 10^{-4}$ should be valid, where $\omega$ is the frequency of the electromagnetic radiation and $\Delta\omega$ is the deviation from the Bragg angle for the given angle of incidence.

In X-ray diffraction optics [1] crystal monochromators are common used to obtain radiation with given angular and spectral properties. In that case, according to Bragg or Laue the radiation from the source is first reflected from one or two crystal monochromators and then it is incident on the studied sample. As a rule, two-wave scattering is used in all the crystals, i.e. diffracted reflection takes place in each crystal from any system of crystal planes. In this case, in order to obtain a parallel and monochromatic beam it is necessary that the beam be reflected at least from two crystals, since according to Bragg one crystal sets only a mutually unique correspondence between the frequency and the direction of radiation propagation.

The set-up with three crystals, however, proves to be rather complicated because while adjusting them a high accuracy in the mutual spatial positions of all the crystals is necessary. For that reason spectrometers with four crystals are not used practically, though a four-crystal set-up is more advantageous as it may secure a good angular direction and monochromatization of the beam without changing its initial direction.

[1]) Mravyan-1, Erevan 49, USSR.

A new arrangement of a crystal monochromator with three-wave Bragg diffraction is offered in this work, which allows to make feasible spectrometer arrangement with four crystals. In it instead of three initial crystals used as monochromators three sets of reflecting planes of the same crystal are utilized. If in the crystalline sample three-wave scattering is being analyzed, the most convenient case is the so-called coplanar one, when the wave vectors $\boldsymbol{k}_0$ of the incident and $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ of the two diffracted waves are in the same plane. In this case the crystal monochromator represents three vertical blocks on a common basis [2]. The general view of a monochromator is shown in Fig. 1, the plane of diffraction in which the wave vectors $\boldsymbol{k}_0$, $\boldsymbol{k}_1$, $\boldsymbol{k}_2$ lie is parallel to the base. As the three blocks are cut out of the same crystal the beam reflected by the first block is automatically in Bragg direction with reference to the second block, etc. Let $\boldsymbol{h}_1$, $\boldsymbol{h}_2$ be vectors of reflecting sets of planes of the reciprocal lattice. Here we have $\boldsymbol{k}_1 = \boldsymbol{k}_0 + \boldsymbol{h}_1$, $\boldsymbol{k}_2 = \boldsymbol{k}_0 + \boldsymbol{h}_2$. For a three-wave diffraction to be realized it is necessary that the incident wave vector satisfies Bragg conditions for two sets of planes simultaneously, that is $k_1^2 \approx k_2^2 \approx k_0^2$. In the coplanar case this is possible only for a definite wavelength of radiation:

$$\lambda_m = \frac{4\pi \sin \varphi}{|\boldsymbol{h}_1 - \boldsymbol{h}_2|}, \tag{1}$$

where $\varphi$ is the angle between the vectors $\boldsymbol{h}_1$ and $\boldsymbol{h}_2$. Thus the three-wave crystal monochromator cuts a narrow range from the continuous spectrum of the synchrotron radiation near $\lambda_m$. It is to be noticed that $\lambda_m$ can be changed by choosing the vectors $\boldsymbol{h}_1$ and $\boldsymbol{h}_2$.

In the symmetrical case, when $|\boldsymbol{h}_1| = |\boldsymbol{h}_2| = |\boldsymbol{h}_1 - \boldsymbol{h}_2|$, the path of rays in the monochromator is illustrated in Fig. 2. The plane wave with wave vector $\boldsymbol{k}_0$ is incident normally on the surface of the first block. Two reflected waves with wave vectors $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ emerge from that surface. The ray with wave vector $\boldsymbol{k}_1$ is incident on the second block from which the wave vector $\boldsymbol{k}_2$ emerges and is incident on the third block. In the third block one of the two diffracted waves has again a wave vector nearly equal to $\boldsymbol{k}_0$.

The greatest interest offers the angular and frequency dependences of the transmission coefficient $R$ (total reflection coefficient). The analysis of these dependence needs the application of the three-wave X-ray diffraction theory; practically it cannot be carried out analytically for an arbitrary angular orientation of the incident beam because in that case for determining the dispersive corrections it is necessary to solve an equation of sixth degree. On the other hand, a numerical calculation of the problem by electronic computors offers no principal difficulty, as the computation methods of linear algebra are highly developed (see, e.g., [3]). The general formulation of the dynamic theory of multiwave Bragg reflection in a form of maximum convenience for the application of the computation methods is given in [4].

Introduce a vector $\boldsymbol{\varkappa}_0$ with modulus $|\boldsymbol{\varkappa}_0| = \omega_0/c = 2\pi/\lambda_m$ the direction of which coincides strictly with the Bragg direction for the frequency $\omega_0$, i.e.

$$(\boldsymbol{\varkappa}_0 + \boldsymbol{h}_1)^2 = (\boldsymbol{\varkappa}_0 + \boldsymbol{h}_2)^2 = \varkappa_0^2 . \tag{2}$$

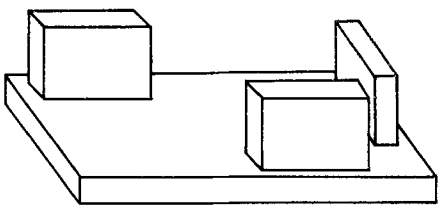

Fig. 1. General view of crystal monochromator

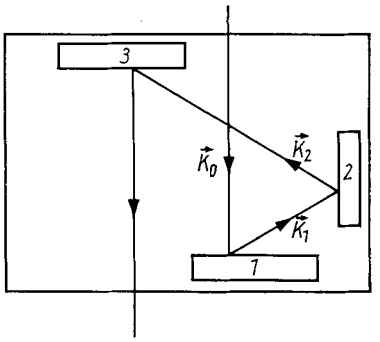


Fig. 2. Path of rays into the monochromator

The wave vector $\boldsymbol{k}_0$ may slightly differ from $\boldsymbol{\varkappa}_0$ both in direction and magnitude. Write

$$\boldsymbol{k}_0 = \boldsymbol{\varkappa}_0 + \boldsymbol{q}_0; \qquad \boldsymbol{q}_0 = \varkappa_0(\theta_1 \boldsymbol{e}_{0\pi} + \theta_2 \boldsymbol{e}_{0\sigma} + \theta_\omega \boldsymbol{s}_0)\,, \tag{3}$$

where $\boldsymbol{s}_0$ is a unit vector parallel to $\boldsymbol{\varkappa}_0$, $\boldsymbol{e}_{0\sigma}$ a unit vector parallel to $(\boldsymbol{h}_1 - \boldsymbol{h}_2)$, $\boldsymbol{e}_{0\pi} = [\boldsymbol{e}_{0\sigma} \times \boldsymbol{s}_0]$, $\theta_\omega = (\omega - \omega_0)/\omega_0$.

In the considered coplanar case the electric field amplitude of the wave which has passed through the monochromator depends only on $\theta_2$ and $\theta_\omega$ and does not depend on $\theta_1$ in the linear $\theta$ approximation by analogy to two-wave diffraction. Just as in the two-wave case, the direction of the electric field vector of the incident wave $\boldsymbol{E}^{(\mathrm{in})}$ passing through the monochromator is preserved if the vector $\boldsymbol{E}^{(\mathrm{in})}$ is parallel to one of two vectors of the standard polarization $\boldsymbol{e}_{0\pi}$ and $\boldsymbol{e}_{0\sigma}$. The projections of the vectors of the incident electric field $\boldsymbol{E}^{(\mathrm{in})}$ and of the transmitted wave $\boldsymbol{E}^{(\mathrm{out})}$ on the vector $\boldsymbol{e}_{0s}(s = \pi, \sigma)$ are correlated by

$$(\boldsymbol{e}_{0s}\boldsymbol{E}^{(\mathrm{out})}) = P^{ss}_{123}(\theta_2, \theta_\omega)\,(\boldsymbol{e}_{0s}\boldsymbol{E}^{(\mathrm{in})})\,, \tag{4}$$

where we have dropped an unessential phase multiplier, defining the dependence on coordinates.

The diagonal matrix of the transition $P^{ss}_{123}$ is explained in [4]. It represents a product of three diagonal matrices $P^{ss}_m$, each of which corresponds to reflection from the $m$-th block of the monochromator,

$$P^{ss}_{123} = P^{ss}_3 P^{ss}_2 P^{ss}_1\,, \tag{5}$$

and is expressed by eigenvectors of the matrix of dynamic diffraction or, in other words, by the matrix in the system of the basic equation of the dynamical theory. Referring to [4] for details, it is worth noticing here that according to Fig. 2 the matrix $P^{ss}_1$ corresponds to transition of the wave with vector $\boldsymbol{k}_0$ into a wave with vector $\boldsymbol{k}_1 = \boldsymbol{\varkappa}_1 + \boldsymbol{q}_1$, where $\boldsymbol{\varkappa}_1 = \boldsymbol{\varkappa}_0 + \boldsymbol{h}_1$.

In the second reflection the plane wave with vector $\boldsymbol{k}_1$ is the initial one and its scattering is considered in a wave with vector $\boldsymbol{k}_2 = \boldsymbol{\varkappa}_2 + \boldsymbol{q}_2$, where $\boldsymbol{\varkappa}_2 = \boldsymbol{\varkappa}_0 + \boldsymbol{h}_2$. In this case the angular declination from the strict Bragg direction $\boldsymbol{\varkappa}_1$ is determined by the vector $\boldsymbol{q}_1 = \boldsymbol{q}_0 - \boldsymbol{n}_1(\boldsymbol{h}_1\boldsymbol{q}_0)/(\boldsymbol{\varkappa}_1\boldsymbol{n}_1)$, where $\boldsymbol{n}_1$ is the vector of the inner normal, directed to the entrance surface of the first block. It should be noted that the vector $\boldsymbol{q}_1$ differs from $\boldsymbol{q}_0$ only by a normal vector to the reflecting surface $\boldsymbol{n}_1$, and besides $\boldsymbol{\varkappa}_0\boldsymbol{q}_0 = \boldsymbol{\varkappa}_1\boldsymbol{q}_1$. These conditions permit to form the vector $\boldsymbol{q}_1$ geometrically in a relatively simple way. It is easy to be convinced that resolving the vector $\boldsymbol{q}_1$ on the basis $\boldsymbol{e}_{1\pi}$, $\boldsymbol{e}_{1\sigma}$, $\boldsymbol{s}_1$, correlated with the vector $\boldsymbol{\varkappa}_1$ and determining the new values of the parameters of $\theta^{(1)}_2$ and $\theta^{(1)}_\omega$, then $\theta^{(1)}_\omega = \theta_\omega$; as is the case of elastic scattering, but $\theta^{(1)}_2 \neq \theta_2$, because of the asymmetrical reflection. The calculation of the vectors $\boldsymbol{q}_2$, $\boldsymbol{q}_3$, and of the matrix $P^{ss}_3$ is carried out analogously. After the third reflection $\boldsymbol{\varkappa}_3 = \boldsymbol{\varkappa}_0$, but $\boldsymbol{q}_3 \neq \boldsymbol{q}_0$: $\sigma$ is the projection of $\boldsymbol{q}_3$ and consequently $\boldsymbol{k}_3$ changes its sign.

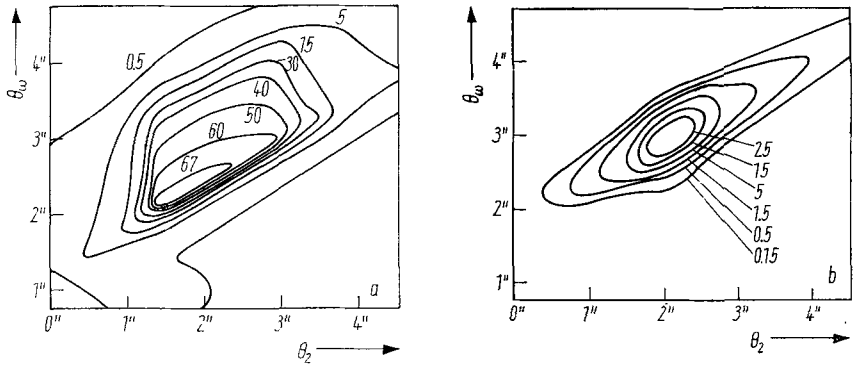


Fig. 3. Total reflection coefficient for a) $\pi$-polarization and b) $\sigma$-polarization

The reflection coefficient $R_s$ for polarization $S$ is defined in the following way:

$$R_s(\theta_2, \theta_\omega) = |P^{ss}_{123}(\theta_2, \theta_\omega)|^2 . \tag{6}$$

Concrete numerical calculations of these quantities were carried out for the case (044/440) of three-wave diffraction in silicon. In this case $\lambda_m = 1.663$ Å, that is very close to the wavelength of $NiK_\alpha$ radiation. The results of the calculation are represented in Fig. 3. The calculation was carried out for the region $0.75'' \leqq \theta_\omega \leqq 4.75''$, $0 \leqq \theta_2 \leqq 4.5''$. First of all one must note the extremely great value ($\approx 70\%$) of the maximum of the total reflection coefficient for $\pi$-polarization (Fig. 3a). It is caused by the fact that in this case practically only two of the three reflections are three-wave ones. The side reflection is a two-wave one, as the wave with the wave vector directed along the surface of the block is not excited. Therefore, its reflection coefficient is close to unity. As for the three-wave reflections, since in fact the maximum reflection is removed from the centre of the three-wave region, the value of the reflection coefficient is also greater than 0.5.

The calculations show that the considered arrangement of reflecting surface blocks is extremely effective when it is used as monochromator in two-wave experiments. Its advantages are the relative simplicity (of one crystal), compactness, an extreme monochromaticity and angular direction of the leaving radiation having enough intensity in the necessary range of angles and frequencies.

## References

[1] Z. G. PINSKER, Dynamical Scattering of X-Rays in Crystals, Springer-Verlag, 1978.
[2] R. Z. GABRIELYAN, P. A. BEZIRGANYAN, and F. O. EIRAMSHYAN, Dokl. Akad. Nauk Arm. SSR **64**, 38 (1977); phys. stat. sol. (a) **43**, K183 (1977).
[3] J. H. WILKINSON and C. REINSCH, Handbook for Automatic Computation, Linear Algebra, Springer-Verlag, Berlin 1976.
[4] V. G. KOHN, phys. stat. sol. (a) **54**, 375 (1979).

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